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On the Extreme Points of a Certain Convex Polytope*

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ABSTRACT

The convex polytope of all stochastic and symmetric matrices is considered and its extreme points are determined. A method is given for counting these extreme points.

1. INTRODUCTION

A $n \times n$ matrix is said to be doubly stochastic (d.s.) if its elements are non-negative and the sum of the elements in each row and column is equal to 1. Denote by Δ_n the convex polytope of all d.s. matrices. A well-known result to Birkhoff [2] states: (i) every $n \times n$ permutation matrix is an extreme point of Δ_n, (ii) every d.s. matrix is a convex combination of permutation matrices. Both (i) and (ii) show that the $n!$ permutation matrices are the extreme points of Δ_n. Part (i) is immediate and part (ii) can be deduced from a result of König-Frobenius [2] which states that every d.s. matrix contains a positive diagonal, i.e., there exists a permutation π of the numbers from 1 to n such that $a_{i\pi(i)} > 0$, $1 \leqslant i \leqslant n$.

We consider the convex polytope Γ_n of all stochastic and symmetric matrices, i.e., the convex set of all matrices $(x_{ij})_1^n$ the elements of which satisfy

$$x_{ij} \geqslant 0, \qquad \sum_{j=1}^{n} x_{ij} = 1, \qquad x_{ij} = x_{ji}, \qquad i, j = 1, 2,..., n.$$

Clearly $\Gamma_n \subset \Delta_n$ and we ask whether Γ_n has extreme points other than the symmetric permutation matrices. The answer to this question is

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positive. In our main result (Theorem 1) we give a construction of the set of the extreme points of Γ_n. At the end (Theorem 2) we give a method for counting these extreme points and determine their number for Γ_4, Γ_5 and Γ_6.

2. Construction of the Set Σ_n of Extreme Points

Consider a permutation π of all the natural numbers from 1 to n and denote by P the corresponding permutation matrix. Clearly P is symmetric if and only if π can be resolved into cycles of length 1 and 2 only. Let now $\pi = \sigma_1\sigma_2 \cdots \sigma_r$ be a permutation of the numbers from 1 to n resolved into its disjoint cycles and assume that at least one of its cycles $\sigma = (ab... kl)$ is of length $s > 2$. We construct a matrix A of order s in the following manner. The positive elements of A are situated only in the places

$$(a, b), (b, c),..., (k, l), (l, a) \tag{1}$$

$$(b, a), (c, b),..., (l, k), (a, l) \tag{2}$$

Let us assume first that s is even. Then for each α, $0 < \alpha < 1$, we construct the matrix $A = A(\sigma, \alpha)$ of Γ_s in the following way. We put the number α into the places (a, b) and (b, a) of A. Hence we have to put $1 - \alpha$ into the places (c, b) and (b, c). Continuing in this way, we see that the matrix $A(\sigma, \alpha)$ is defined by having the value α in the places

$$(a, b), (b, a), (c, d), (d, c),..., (k, l), (l, k) \tag{3}$$

and the value $1 - \alpha$ in the places

$$(b, c), (c, b),..., (l, a), (a, l) \tag{4}$$

Hence we obtain

$$A(\sigma, \alpha) = \alpha P_s' + (1 - \alpha) P_s'', \tag{5}$$

where P_s' is a symmetric permutation matrix of order s having the ones in the positions (3) and P_s'' is a symmetric permutation matrix having the ones in the positions (4). The equality (5) shows that $A(\sigma, \alpha)$ is not an extreme point of Γ_s.

We consider now the case in which the length s of the cycle $\sigma = (ab \cdots kl)$ is odd. Choosing again α, $0 < \alpha < 1$, and starting as in the former case, we put the value α into the places (a, b) and (b, a) of $A \in \Gamma_s$. This time, however, α appears in the place (a, l) and also in the place (l, a), hence

$\alpha = 1/2$. For such a cycle σ of odd length $s > 1$, we denote the matrix $A(\sigma, 1/2)$ by $S(\sigma)$.

LEMMA 1. *$S(\sigma)$ is an extreme point of Γ_s.*

PROOF: Let us assume that

$$S(\sigma) = \alpha A + (1 - \alpha) B \tag{6}$$

where $0 < \alpha < 1$ and A and B belong to Γ_s. The matrix A cannot be a symmetric permutation matrix. For, suppose that A is a symmetric permutation matrix; then the corresponding permutation $\pi(\sigma)$ of the numbers $a, b, \ldots, l$ contains cycles of length 1 and 2 only. But $S(\sigma)$ does not contain positive elements on the main diagonal. Hence $\pi(\sigma)$ contains cycles of length 2 only and thus the order s of A is even, in contradiction to the assumption that s is odd.

As $A \in \Gamma_s$ is not a symmetric permutation matrix, it follows that A contains a row, say row a, in which there are at least two positive elements. By (6) the row a of A can contain positive elements only in the places (a, b) and (a, l). Hence we have to put positive elements also in the places (b, a) and (l, a). Continuing this way, we see that A has positive elements exactly at the $2s$ places (1) and (2). But we have shown above that this implies that all these positive elements are of value $1/2$; hence $A = S(\sigma)$ and $S(\sigma)$ is thus an extreme point of Γ_s.

After these preparations we now construct the matrices $S(\pi)$ of Γ_n. Let $\pi = \sigma_1 \cdots \sigma_r$ be a permutation of the numbers from 1 to n resolved into its disjoint cycles. If (m) is a cycle of length 1, we put 1 in the position (m, m) (and therefore zeros in all other places of the m-th row and column). If σ is the cycle $(m\,n)$, we put 1 in the places (m, n) and (n, m). If $\sigma = (ab \cdots kl)$ is of even length, we put 1 either in all the positions (3) or in all the positions (4). (Hence in this case π does not define $S(\pi)$ in a unique way.) Finally, if σ is of odd length, we put $1/2$ in all the positions (1) and (2). Given n, we denote the class of these matrices $S(\pi)$ by Σ_n.

LEMMA 2. *Each $S(\pi)$ is an extreme point of Γ_n.*

PROOF: The cycles containing the ones determine symmetric permutation matrices (of dimension equal to the length of the cycle). Hence they are extreme by virtue of Birkhoff's theorem and the odd cycles containing the halves cannot be written as convex combination of symmetric d.s. matrices, as we have shown above. As for each cycle σ of π the corresponding matrix is extreme in Γ_s, it follows that $S(\pi)$ is extreme in Γ_n.

We conclude this section with some examples.

$n = 3$: The only extreme point of Γ_3, different from the 4 symmetric permutation matrices is the following:

$$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix},$$

which corresponds to $\pi = (123)$.

$n = 4$:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix},$$

which corresponds to $\pi = (1)(234)$.

$n = 5$:

$$\begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

The first matrix corresponds to $\pi = (12534)$ and the second to $\pi = (1\ 2\ 3)(4\ 5)$.

3. Proof That Each Extreme Point Belongs to Σ_n

LEMMA 3. *Each matrix A of Γ_n is a convex combination of matrices $S(\pi) \in \Sigma_n$.*

PROOF: By the result of König-Frobenius mentioned above, A possesses a positive diagonal $a_{i\pi(i)} > 0$, $1 \leqslant i \leqslant n$. Denote as above the resolution of π into disjoint cycles by $\pi = \sigma_1 \cdots \sigma_r$ and let $S = S(\pi)$ be a corresponding extreme point. (If no cycle σ is of even length larger than 2, $S(\pi)$ is uniquely determined.) By the symmetry of A, to every odd cycle σ correspond the elements in the places (1) and (2). Denote by u the minimal element of them, the minimum being taken relative to all odd cycles σ of π of length larger than 1. Similarly, to every even cycle correspond elements of A in the places (3) or (4) and to every cycle of length 1 corresponds an element of A on the main diagonal. Denote again by t the minimum of all these elements, the minimum being taken relative to all the cycles of length 1 and all the cycles of even length. We distinguish between the following two cases:

(a) $t \leqslant 2u$. Then

$$B = \frac{A - tS}{1 - t}$$

belongs to Γ_n and has at least one positive element less than A. It follows that $A = tS + (1 - t) B$ and the process can be repeated with B. If $t = 1$, then $u = 1/2$ and on account of the minimality of u, $A \in \Sigma_n$.

(b) $t > 2u$. Then

$$C = \frac{A - 2uS}{1 - 2u}$$

also belongs to Γ_n and has at least two positive elements less than A. If $u = 1/2$, then all the elements of A corresponding to the odd cycles σ of π are equal to $1/2$ and, by the assumption $t > 2u$, π does not contain cycles of length 1 or of even length. Hence $u = 1/2$ implies $A \in \Sigma_n$. This concludes the proof.

The Lemmas 1, 2, and 3 establish our main result.

THEOREM 1. *Σ_n is the set of all the extreme points of Γ_n.*

4. NUMBER OF EXTREME POINTS

Our aim now is to count the extreme points of Γ_n. Following [1] we shall consider the class α of permutations having α_1 cycles of length 1, α_2 cycles of length 2, and generally α_i cycles of length i, where i takes all the odd values from 3 to n if n is odd, or to $n - 1$ if n is even. Here we take into account the fact that all even cycles $(ab \cdots kl)$ of length larger than 2, by the transition from the positions (1) and (2) to the positions (3) and (4), were reduced to cycles of length 2. The numbers α_i satisfy the equality

$$\alpha_1 + 2\alpha_2 + \cdots + n\alpha_n = n, \qquad \text{if} \quad n \text{ is odd,}$$

and

$$\alpha_1 + 2\alpha_2 + \cdots + (n - 1)\, \alpha_{n-1} = n, \qquad \text{if} \quad n \text{ is even.}$$

The number of all distinct permutations of this class is

$$h_\alpha = \frac{n!}{1^{\alpha_1}\alpha_1!\,2^{\alpha_2}\alpha_2!\cdots n^{\alpha_n}\alpha_n!}, \qquad \text{if } n \text{ is odd,}$$

and

$$h_\alpha = \frac{n!}{1^{\alpha_1}\alpha_1!\,2^{\alpha_2}\alpha_2!\cdots (n-1)^{\alpha_{n-1}}\alpha_{n-1}!}, \qquad \text{if } n \text{ is even.}$$

Now, every matrix $S(\sigma)$, corresponding to the odd cycle σ, by (1) and (2) corresponds also to the inverse cycle σ^{-1}. Therefore, to every class α correspond $h_\alpha/2^p$ extreme points, where p is the number of odd cycles of length larger than 1, appearing in this class. Thus we proved the following

THEOREM 2. *The number of all the extreme points of Γ_n is equal to the sum of all $h_\alpha/2^p$, corresponding to all the classes of permutations α described above.*

We have seen that Γ_3 contains 5 extreme points. We now count the extreme points of Γ_4, Γ_5, and Γ_6:

Γ_4

$\alpha_1 = 4$		$h_\alpha = 1$
$\alpha_1 = 2$,	$\alpha_2 = 1$	$h_\alpha = 6$
$\alpha_1 = 1$,	$\alpha_3 = 1$	$h_\alpha/2 = 4$
$\alpha_2 = 2$		$h_\alpha = 3$

Γ_5

$\alpha_1 = 5$		$h_\alpha = 1$
$\alpha_1 = 1$,	$\alpha_2 = 2$	$h_\alpha = 15$
$\alpha_1 = 2$,	$\alpha_3 = 1$	$h_\alpha/2 = 10$
$\alpha_2 = 1$,	$\alpha_3 = 1$	$h_\alpha/2 = 10$
$\alpha_5 = 1$,		$h_\alpha/2 = 12$
$\alpha_1 = 3$,	$\alpha_2 = 1$	$h_\alpha = 10$

Γ_6

$\alpha_1 = 6$			$h_\alpha = 1$
$\alpha_1 = 4$,	$\alpha_2 = 1$		$h_\alpha = 15$
$\alpha_1 = 3$,	$\alpha_3 = 1$		$h_\alpha/2 = 20$
$\alpha_1 = 2$,	$\alpha_2 = 2$		$h_\alpha = 45$
$\alpha_1 = 1$,	$\alpha_2 = 1$,	$\alpha_3 = 1$	$h_\alpha/2 = 60$
$\alpha_1 = 1$,	$\alpha_5 = 1$		$h_\alpha/2 = 72$
$\alpha_2 = 3$			$h_\alpha = 15$
$\alpha_3 = 2$			$h_\alpha/4 = 10$

We obtained 14 extreme points for Γ_4, 58 extreme points for Γ_5, and 238 extreme points for Γ_6.

We conclude with the following remark. In [3], Mirsky determined the set of extreme points for the polytope of all doubly substochastic matrices. Using his methods it can be shown that the analogous result holds also for the polytope of all symmetric substochastic matrices. Denote by $\Sigma_n{}^0$ the set consisting of all the matrices of Σ_n and all matrices of Σ_n where some ones at symmetric places or on the main diagonal are replaced by zeros. Then $\Sigma_n{}^0$ *is the desired set of extreme points.*

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